

# Skeleton series and multivaluedness of the self-energy functional in zero space-time dimensions

Riccardo Rossi<sup>1</sup> and Félix Werner<sup>2</sup>  
*Laboratoire de Physique Statistique<sup>1</sup> and Laboratoire Kastler Brossel<sup>2</sup>,  
 Ecole Normale Supérieure, UPMC, Université Paris Diderot<sup>1</sup>,  
 Collège de France<sup>2</sup>, CNRS, 24 rue Lhomond, 75005 Paris, France*

Recently, Kozik, Ferrero and Georges have discovered numerically that for a family of fundamental models of interacting fermions, the self-energy  $\Sigma[G]$  is a multi-valued functional of the fully dressed single-particle propagator  $G$ , and that the skeleton diagrammatic series  $\Sigma_{\text{bold}}[G]$  converges to the wrong branch above a critical interaction strength. We consider the zero space-time dimensional case, where the same mathematical phenomena appear from elementary algebra. We also find a similar phenomenology for the fully bold formalism built on fully dressed single-particle propagator and pair propagator.

In quantum many-body physics, an important role is played by the self-consistent field-theoretical formalism, where the self-energy  $\Sigma$  is expressed in terms of the exact propagator  $G$  (see, *e.g.*, [1] and Refs. therein). In a recent article, Kozik, Ferrero and Georges numerically discovered mathematical difficulties with this formalism [2]. They studied not only the Hubbard model in two space dimensions, but also simpler models—the Hubbard atom and the Anderson impurity model—for which there is no spatial coordinate. Here we consider an even simpler toy-model for which there is no imaginary-time coordinate either. This idea was also followed in the very recent article [3]. For fermionic many-body problems, the partition function can be written as a functional integral over Grassmann fields in  $(d+1)$  space-time dimensions ( $d$  spatial coordinates and one imaginary-time coordinate) [4]. Accordingly, we consider the zero space-time dimensional model defined by a “partition function” given by a simple Grassmann integral,

$$Z = \int \left( \prod_{\sigma} d\varphi_{\sigma} d\bar{\varphi}_{\sigma} \right) e^{-S[\bar{\varphi}_{\sigma}, \varphi_{\sigma}]} \quad (1)$$

with the action

$$S[\bar{\varphi}_{\sigma}, \varphi_{\sigma}] = -\mu \sum_{\sigma} \bar{\varphi}_{\sigma} \varphi_{\sigma} + U \bar{\varphi}_{\uparrow} \varphi_{\uparrow} \bar{\varphi}_{\downarrow} \varphi_{\downarrow}, \quad (2)$$

and a corresponding propagator

$$G = \langle \bar{\varphi}_{\sigma} \varphi_{\sigma} \rangle = \frac{1}{Z} \int \left( \prod_{\sigma} d\varphi_{\sigma} d\bar{\varphi}_{\sigma} \right) e^{-S[\bar{\varphi}_{\sigma}, \varphi_{\sigma}]} \bar{\varphi}_{\sigma} \varphi_{\sigma}. \quad (3)$$

Here  $\sigma \in \{\uparrow, \downarrow\}$  is the spin index, while  $\mu$  and  $U$  are dimensionless parameters that play the roles of chemical potential and interaction strength. Diagrammatically, the Feynman rules for the present toy-model are analogous to the ones of the physical  $(d+1)$  dimensional models, with the simplification that space-time variables are absent and that the propagators are constants.

In this exactly solvable toy-model, we observe a similar phenomenology than the one found by Kozik *et al.* in non-zero space-time dimensions. More precisely, restricting to  $U < 0$ , we find that:

- The mapping  $G_0 \mapsto G(G_0, U)$  is two-to-one and hence the function  $G \mapsto \Sigma(G, U)$  has two branches.
- The skeleton series  $\Sigma_{\text{bold}}(G, U)$ , evaluated at the exact  $G(\mu, U)$ , converges to the correct branch for  $|U| < \mu^2$ , and to the wrong branch for  $|U| > \mu^2$ .

This can be derived very directly from the above definitions. Expanding the exponentials in Eqs. (1,3) yields

$$Z(\mu, U) = \mu^2 - U \quad (4)$$

$$G(\mu, U) = \frac{\mu}{\mu^2 - U}. \quad (5)$$

The propagator for  $U = 0$  is

$$G_0(\mu) = \frac{1}{\mu}. \quad (6)$$

The self-energy  $\Sigma$ , defined as usual by the Dyson equation  $G^{-1} = G_0^{-1} - \Sigma$ , reads

$$\Sigma(\mu, U) = \frac{U}{\mu}. \quad (7)$$

We note that for  $U > 0$ , an obvious pathology appears in this model around  $U = \mu^2$ ; namely,  $Z$  changes sign, and  $G$  diverges. Therefore we restrict to  $U < 0$ .

Eliminating  $\mu$  between Eqs. (5,6) gives

$$G(G_0, U) = \frac{G_0}{1 - U G_0^2}. \quad (8)$$

The map  $G_0 \mapsto G(G_0, U)$  is two-to-one, because the  $G_0$ 's that correspond to a given  $G$  are the solutions of the second order equation

$$U G G_0^2 + G_0 - G = 0, \quad (9)$$

which has the two solutions

$$G_0^{(\pm)}(G, U) = \frac{-1 \pm \sqrt{1 + 4 U G^2}}{2 U G}. \quad (10)$$

These solutions are real provided  $(G, U)$  belongs to the physical manifold  $\{(G(\mu, U), U)\}$ ; indeed,

$$4|U|G(\mu, U)^2 \leq 1. \quad (11)$$

The corresponding self-energies (given by the Dyson equation) are

$$\Sigma^{(\pm)}(G, U) = \frac{-1 \pm \sqrt{1 + 4 U G^2}}{2 G}. \quad (12)$$

The correct self-energy  $\Sigma(\mu, U)$  is recovered from  $\Sigma^{(s)}(G(\mu, U), U)$  provided one takes the determination

$$s = \text{sign}(\mu^2 - |U|). \quad (13)$$

We turn to a discussion of the skeleton diagrammatic series  $\Sigma_{\text{bold}}(G, U)$  for the self-energy  $\Sigma$  in terms of fully dressed propagator  $G$  and bare vertex  $U$ . We find that  $\Sigma_{\text{bold}}(G, U)$  is the  $U \rightarrow 0$  Taylor series of  $\Sigma^{(+)}(G, U)$ . Before deriving this, we note that obviously,  $\Sigma_{\text{bold}}(G, U)$  can never be the Taylor series of  $\Sigma^{(-)}(G, U)$ , since the former vanishes at  $U = 0$  while the latter does not. For the derivation, it is convenient to introduce  $g := \sqrt{|U|} G$  and  $g_0 := \sqrt{|U|} G_0$ , so that Eqs.(8,10) simplify to  $g(g_0) = g_0/(1 + g_0^2)$  and  $g_0^{(\pm)}(g) = (1 \mp \sqrt{1 - 4g^2})/(2g)$ . The key point is that  $g_0^{(+)}(g(g_0)) \hat{=} g_0$ , where the symbol  $\hat{=}$  means equality in the sense of formal power series. This is because the inverse mapping of  $g(g_0)$  is  $g_0^{(+)}(g)$  for small  $g_0$  and  $g$ . Let us then denote by  $\Sigma_{\text{bare}}(G_0, U)$  the diagrammatic series for the self-energy in terms of bare propagators and vertices. Setting  $\Sigma_{\text{bold}}(G, U) =: \sqrt{|U|} \sigma_{\text{bold}}(g)$  and  $\Sigma_{\text{bare}}(G_0, U) =: \sqrt{|U|} \sigma_{\text{bare}}(g_0)$ , a defining property of  $\sigma_{\text{bold}}$  is that  $\sigma_{\text{bold}}(g(g_0)) \hat{=} \sigma_{\text{bare}}(g_0)$ . In the present toy-model, we simply have  $\Sigma_{\text{bare}}(G_0, U) = U G_0$ , *i.e.*,  $\sigma_{\text{bare}}(g_0) = -g_0$ . Hence,  $\sigma_{\text{bold}}(g) \hat{=} -g_0^{(+)}(g)$ , *i.e.*,  $\Sigma_{\text{bold}}(G, U) \hat{=} U G_0^{(+)}(G, U) = \Sigma^{(+)}(G, U)$ .

Explicitly, expanding the square root in Eq. (12) yields

$$\Sigma_{\text{bold}}(G, U) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1} (2n-2)!}{n! (n-1)!} G^{2n-1} U^n. \quad (14)$$

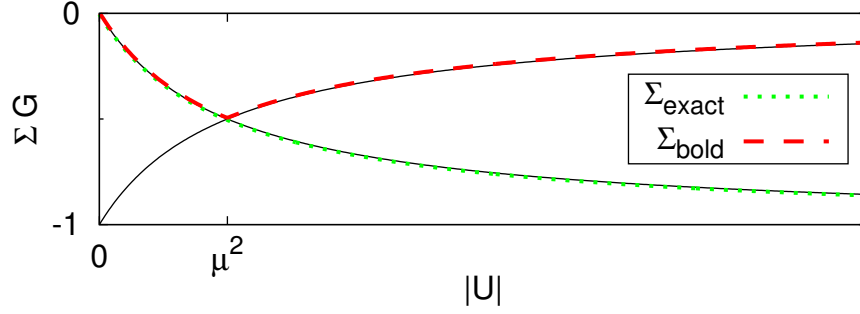


FIG. 1. The two branches of the self-energy  $\Sigma$ , multiplied for convenience by  $G$ , as a function of the interaction strength  $|U|$ , for fixed  $\mu$ . Dotted line: exact self-energy  $\Sigma_{\text{exact}} = \Sigma(\mu, U)$ , dashed line: skeleton series  $\Sigma_{\text{bold}}(G, U)$ . The upper branch corresponds to  $\Sigma^{(+)}(G, U)$ , the lower branch to  $\Sigma^{(-)}(G, U)$ . Here,  $G$  stands for the exact  $G(\mu, U)$ .

It is natural to evaluate the bold series at the exact  $G(\mu, U)$ . The obtained series always converges, as follows from the inequality (11). The convergence is always to  $\Sigma^{(+)}(G(\mu, U), U)$ , which as we have seen is the correct result for  $|U| < \mu^2$ , and the wrong one for  $|U| > \mu^2$ . The convergence speed is slow for  $|U|$  close to  $\mu^2$ , and gets faster not only in the small  $|U|$  limit, but also in the large  $|U|$  limit. This is qualitatively identical to the numerical observations of Kozik *et al.* in non-zero space-time dimensions. We note that the series converges even at the critical value  $|U| = \mu^2$ , albeit very slowly (the summand behaving as  $1/n^{3/2}$  for large  $n$ ); at this point, the boundary of the series' convergence disc is reached.

In the Figure we plot the quantity  $\Sigma G$ , which, for the exact  $\Sigma$ , is equal to  $U$  times the double occupancy  $\langle \bar{\varphi}_{\uparrow} \varphi_{\uparrow} \bar{\varphi}_{\downarrow} \varphi_{\downarrow} \rangle$ , versus  $|U|$  for fixed  $\mu$ . The picture is qualitatively identical to Fig. 2(a) of Kozik *et al.*

Geometrically, the mapping  $U \mapsto \Sigma(G, U)$  can be viewed as single-valued on a two-sheeted Riemann-surface with a branch point at  $-1/(4G^2)$ . Let us vary  $U$  from 0 to  $-\infty$  for fixed  $\mu$ . For small  $|U|$ , the point  $U$  is far away from the branch point and the bold series converges quickly. The result corresponds to the correct Riemann-sheet. Upon increasing  $|U|$ , the point  $U$  and the branch point  $-1/(4G^2(\mu, U))$  both move leftwards. The point  $U$  catches up the branch point when  $|U| = \mu^2$ . For larger  $|U|$ ,  $U$  is again to the right of the branch point, and the bold series converges again, but the result corresponds to the wrong sheet. In principle, the correct result can be recovered from  $\Sigma_{\text{bold}}(G, U)$  by analytic continuation along a path where  $U$  rotates once around the branch point.

As emphasized by Kozik *et al.*, since the self-energy is the functional derivative of the Luttinger-Ward functional  $\Phi[G, U]$  with respect to  $G$ , and since  $\Sigma[G, U]$  is multivalued,  $\Phi$  must also be multivalued. This can also be seen explicitly in the present model. The Luttinger-Ward functional (which is actually a function in the present model) can be constructed following the usual procedure (see, *e.g.*, [1]). Starting from the free energy  $F(\mu, U) = -\ln Z(\mu, U)$ , and noting that

$$\frac{\partial F}{\partial \mu}(\mu, U) = -2G, \quad (15)$$

the Baym-Kadanoff functional is defined by Legendre transformation:

$$\Omega(G, U) = F(\mu, U) + 2\mu G \quad (16)$$

with  $\mu(G, U)$  such that Eq. (15) holds. The Luttinger-Ward functional is then defined by

$$\Phi(G, U) = \Omega(G, U) - \Omega(G, 0). \quad (17)$$

This leads to the expression

$$\Phi_{\pm}(G, U) = -\ln |\Sigma^{(\mp)}(G, U)| - \ln |G| - 2G \Sigma^{(\mp)}(G, U) - 2. \quad (18)$$

There are two branches because Eq. (15) has two solutions. Accordingly, the mapping  $\mu \mapsto F(\mu, U)$  is neither convex nor concave. Finally one can check that<sup>1</sup>

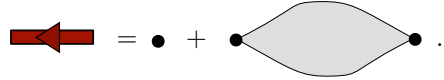
$$\frac{\partial \Phi_{\pm}}{\partial G}(G, U) = 2 \Sigma^{(\pm)}(G, U). \quad (19)$$

We point out that in the present zero space-time dimensional model, both branches  $G_0^{(\pm)}(G, U)$  are physical in the sense that they are the non-interacting propagator for certain parameters of the model. This is not the case for the Hubbard atom and the Hubbard model [2]. More generally, the absence of imaginary-time coordinate constitutes a drastic simplification, and while we have observed similar phenomena than in [2], it remains an open question to which extent the underlying mechanisms are similar.

Finally we briefly treat the fully bold formalism built not only on the fully dressed  $G$  but also on the fully dressed pair propagator  $\Gamma$ . This formalism was used, *e.g.*, in Refs. [5, 6]. One defines

$$\Gamma = U - U^2 \langle \varphi_{\downarrow} \varphi_{\uparrow} \bar{\varphi}_{\uparrow} \bar{\varphi}_{\downarrow} \rangle \quad (20)$$

or diagrammatically



$$\text{thick red arrow} = \bullet + \bullet \text{---} \text{grey lens} \text{---} \bullet. \quad (21)$$

The pair self-energy  $\Pi$  is defined by the Dyson equation  $\Gamma^{-1} = U^{-1} - \Pi$ . The dressed  $G$  and  $\Gamma$  are given in terms of the bare  $G_0$  and  $U$  by Eq. (8) and

$$\Gamma = U \frac{1 - 2U G_0^2}{1 - U G_0^2}. \quad (22)$$

Eliminating  $U$  yields a cubic equation for  $G_0$ , which reads

$$\gamma g_0^3 + 2g_0^2 - 3g_0 + 1 = 0 \quad (23)$$

in terms of the rescaled quantities

$$g_0 := G_0/G \quad (24)$$

$$\gamma := \Gamma G^2. \quad (25)$$

In the relevant range  $0 < |\gamma| \leq 2\sqrt{3}/9$  the three solutions are

$$g_0^{(l)} = \frac{2}{3\gamma} \left[ \sqrt{9\gamma + 4} \cos\left(\frac{\theta(\gamma) + 2\pi l}{3}\right) - 1 \right], \quad l \in \{-1, 0, 1\} \quad (26)$$

where  $\theta(\gamma) = \arg(-27\gamma^2 - 54\gamma - 16 - 3i\sqrt{3}|\gamma|\sqrt{4 - 27\gamma^2}) \in (-\pi, \pi)$ . The fully bold diagrammatic series  $\Sigma_{\text{bold}}(G, \Gamma)$  and  $\Pi_{\text{bold}}(G, \Gamma)$ , evaluated at the exact  $G(\mu, U)$  and  $\Gamma(\mu, U)$ , always converge to the  $l = 1$  branch<sup>2</sup>, which coincides with the exact result for  $|U|/\mu^2 < (1 + \sqrt{3})/2$ . Above this critical interaction strength, the exact result is the  $l = -1$  branch, so that the bold series converges to a wrong result. At this critical interaction, the boundary of the series' convergence disc is reached. In summary, a similar phenomenology occurs again.

The consequences for the Bold Diagrammatic Monte Carlo approach [5–9] of the findings of Ref. [2] and of the present work is left for future study.

<sup>1</sup> The unconventional factors 2 in Eqs. (15,16,19) could be removed by working with spin-dependent  $\mu$  and  $G$ .

<sup>2</sup> Explicitly, we have  $\Sigma_{\text{bold}}(G, \Gamma) \doteq [1/g_0^{(+1)}(\gamma) - 1]/G$  and  $\Pi_{\text{bold}}(G, \Gamma) \doteq \Sigma_{\text{bold}}(G, \Gamma)/[G g_0^{(+1)}(\gamma)]$ .

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